Supporting Information

Quantitative Conformationally Sampled Pharmacophore (CSP) for δ Opioid Ligands: Reevaluation of hydrophobic moieties essential for biological activity

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Table S.1. Biological data for the training set compounds extracted from Clark et al, *J. Pharmacol. Exp. Ther.* **1997**, 283, 501-510**.**

Class	Compound	Efficacy[a]	Binding Affinity[b]
High Efficacy	**1**	1	0.45 (0.38-0.54)
	3	0.36	40 (36-44)
	7	1.02	60 (45-80)
	14	0.59	81 (65-99)
	15	0.59	487 (447-531)
	16	0.8	135 (105-174)
	17	0.9	93 (80-109)
Low Efficacy	**2**	0.08	1.6 (1.5-1.8)
	4	0	0.035 (0.032-0.038)
	5	0.12	6.5 (6.0-7.1)
	6	0.18	8.4 (7.3-9.6)
	8	-	0.079 (0.069-0.086)
	9	-	0.037 (0.034-0.042)
	18	0	37 (29-47)

a: Efficacy determined as the maximum stimulation of [^{35}S]GTPγS binding by the ligand/the maximum response by **1**.
b: Ki from the EC50 for inhibition of specific binding of [^{3}H]**4**.

Table S.2. Overlap coefficients (OC) of the pharmacophore parameters for the δ opioid ligands with respect to **1** obtained using the centroids of pharmacophoric groups as pharmacophore points, i) with sampled probability weighting ii) with equal weighting for all points in conformational space.

i) Centroid

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
2	0	0	0.101498	0	0	0	0	0	0
3	0	0	0.000223	0	0	0	0	0	0
4	0	0.079188	0.000068	0.000033	0	0	0.012717	0.003073	0
5	0	0.081597	0.000065	0.000036	0	0	0.013301	0.003507	0
6	0.000426	0.220968	0.005362	0.004085	0.00014	0.000007	0.000269	0.000083	0.000103
7	0.773058	0.87797	0.85552	0.792749	0.783931	0.732025	0.808095	0.776915	0.818682
14	0.057979	0.012894	0.00924	0.045088	0.12039	0.043429	0.007695	0.007547	0.025091
15	0.064469	0.310567	0.029161	0.112793	0.160007	0.022073	0.084499	0.038984	0.049857
16	0.116873	0.256307	0.031605	0.165934	0.168538	0.038826	0.065071	0.041299	0.051961
17	0.00007	0.00079	0.022113	0.000299	0.003776	0.001526	0.000075	0.00003	0.005938

ii) Centroid=

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
2	0	0	0.279236	0	0	0	0	0	0
3	0	0.007501	0.185472	0	0	0	0	0	0.009671
4	0	0.416378	0.143666	0.091504	0	0	0.285345	0.219663	0
5	0	0.410124	0.137348	0.102236	0	0	0.298971	0.228599	0
6	0.1309	0.644167	0.274613	0.324953	0.124757	0.030024	0.193603	0.134542	0.08169
7	0.854702	0.834232	0.832562	0.816605	0.777649	0.763432	0.721643	0.707111	0.770838
14	0.184387	0.223879	0.176604	0.202835	0.323014	0.216088	0.2168	0.267273	0.275495
15	0.210913	0.337819	0.369037	0.256642	0.30895	0.222845	0.240309	0.280767	0.255997
16	0.193221	0.308019	0.351983	0.231614	0.27156	0.193142	0.232551	0.278274	0.241426
17	0.017294	0.09131	0.349935	0.026434	0.110069	0.121093	0.069646	0.040586	0.217898

Table S.3. Overlap coefficients (OC) of the pharmacophore parameters for the δ opioid ligands with respect to **1** obtained using the most distant atoms between pharmacophoric groups, A and B as pharmacophore points, i) with sampled probability weighting ii) with equal weighting for all points in conformational space.

i) MaxD

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
2	0	0	0.007492	0	0	0	0	0	0
3	0	0.000037	0.057046	0	0.000019	0	0	0	0.000529
4	0	0.000297	0.000996	0.001162	0.000008	0.000069	0.050368	0.092267	0
5	0	0.000299	0.001019	0.001205	0.000008	0.000067	0.049747	0.090954	0
6	0.001138	0.006364	0.044116	0.009805	0.001433	0.000086	0.01293	0.003295	0.000063
7	0.877801	0.862521	0.906859	0.863371	0.840738	0.836287	0.84384	0.83369	0.914309
14	0.008131	0.069736	0.074764	0.024668	0.024471	0.002099	0.015398	0.012378	0.021763
15	0.001921	0.01835	0.070327	0.010232	0.009454	0.002889	0.020799	0.00843	0.025072
16	0.064178	0.218799	0.084515	0.125446	0.098641	0.012334	0.02939	0.021944	0.040306
17	0.000028	0.00037	0	0.000062	0.000359	0	0.00015	0.000021	0

ii) MaxD=

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
2	0	0	0.243021	0	0	0	0	0	0
3	0.001318	0.059892	0.425679	0	0.055935	0	0	0	0.254919
4	0.006042	0.121844	0.212793	0.203099	0.022993	0.112956	0.401597	0.387985	0
5	0.006115	0.116242	0.215273	0.199653	0.019161	0.11343	0.410183	0.390259	0
6	0.110273	0.330804	0.352174	0.336659	0.243425	0.144759	0.342702	0.273682	0.128155
7	0.866672	0.860403	0.849798	0.831695	0.843126	0.814867	0.791782	0.791976	0.842678
14	0.277903	0.490142	0.482687	0.341909	0.332659	0.341528	0.335554	0.315107	0.331111
15	0.182369	0.343814	0.41009	0.263747	0.256638	0.278786	0.335672	0.306372	0.284168
16	0.337089	0.422644	0.376865	0.376684	0.364308	0.282081	0.331229	0.33415	0.256687
17	0.027162	0.125897	0	0.047612	0.11537	0	0.1156	0.06036	0

Table S.4. Statistical analysis of regression models with R^2 values 0.9 and greater from Table 2. The values for the regression parameters and the corresponding P-values are listed for the different 2D pharmacophoric parameter OC combinations.

i) Centroid=

2D Pharmacophoric Parameters	R^2	Intercept	Coefficient 1	Coefficient 2	Coefficient 3
NA-NBA + BN-NAB	0.898	0.123	5.029	-2.574	
		0.079	0.002	0.028	
AB-NBA + BN-NAB + NA-NBA	0.904	0.050	0.370	-2.445	4.726
		0.733	0.582	0.053	0.010
NA-NBA + BN-NAB + AB-ANB	0.910	0.107	6.165	-4.916	2.147
		0.150	0.016	0.161	0.447
NA-NBA + BN-NAB + AB-NAB	0.910	0.176	4.591	-2.157	-0.194
		0.103	0.011	0.095	0.453
NA-NBA + BN-NAB + BN-ANB	0.901	0.144	4.712	-2.152	-0.263
		0.142	0.018	0.199	0.715
NA-NBA + BN-NAB + BN-NBA	0.899	0.129	4.675	-2.797	0.746
		0.114	0.046	0.086	0.810
NA-NBA + BN-NAB + NA-ANB	0.912	0.180	4.671	-2.166	-0.384
		0.093	0.008	0.085	0.411
NA-NBA + BN-NAB + NA-NAB	0.905	0.160	4.699	-2.106	-0.352
		0.117	0.010	0.138	0.553

ii) MaxD=

2D Pharmacophoric Parameters	R^2	Intercept	Coefficient 1	Coefficient 2	Coefficient 3
AB-NBA + NA-NBA	0.936	0.910	-3.763	4.512	
		0.0001	0.0002	0.0001	
AB-NBA + BN-ANB + NA-NBA	0.944	0.892	-3.821	0.220	4.455
		0.0003	0.0005	0.4545	0.0003
AB-NBA + BN-NAB + NA-NBA	0.961	0.837	-3.517	0.594	3.831
		0.0002	0.0004	0.1363	0.0010
AB-NBA + BN-NBA + NA-NBA	0.942	0.900	-3.790	0.273	4.359
		0.0003	0.0005	0.4997	0.0005
AB-NBA + AB-ANB + NA-NBA	0.972	0.872	-3.584	0.736	3.840
		0.0001	0.0001	0.0556	0.0003
AB-NBA + AB-NAB + NA-NBA	0.947	0.870	-3.697	0.289	4.194
		0.000	0.000	0.361	0.001
AB-NBA + NA-ANB + NA-NBA	0.936	0.909	-3.763	0.002	4.512
		0.0004	0.0007	0.9942	0.0004
AB-NBA + NA-NAB + NA-NBA	0.936	0.908	-3.770	0.015	4.516
		0.000	0.001	0.953	0.000

Table S.5. Overlap coefficients for the pharmacophoric parameters of **17**, using Phe[4]/ Leu[5] as the hydrophobic group, B. The various measurements of overlap coefficients are shown with the values obtained using Leu[5] labeled B2.

Pharmacophoric Parameter	**AB-ANB**	**AB-NAB**	**AB-NBA**	**BN-ANB**	**BN-NAB**	**BN-NBA**	**NA-ANB**	**NA-NAB**	**NA-NBA**
Centroid	0.00007	0.00079	0.02211	0.00030	0.00378	0.00153	0.00008	0.00003	0.00594
B2-Centroid	0.00200	0.03213	0.18284	0.00417	0.00377	0.00092	0.00698	0.00074	0.01779
Centroid=	0.01729	0.09131	0.34994	0.02643	0.11007	0.12109	0.06965	0.04059	0.21790
B2-Centroid=	0.09617	0.22610	0.32401	0.12879	0.15201	0.15276	0.19293	0.21599	0.23493
MaxD	0.00003	0.00037	0.00000	0.00006	0.00036	0.00000	0.00015	0.00002	0.00000
B2-MaxD	0.00055	0.00189	0.18062	0.00098	0.00215	0.00100	0.02070	0.00430	0.02243
MaxD=	0.02716	0.12590	0.00000	0.04761	0.11537	0.00000	0.11560	0.06036	0.00000
B2-MaxD=	0.07988	0.17780	0.38106	0.12709	0.15114	0.15954	0.35330	0.23011	0.25806

Table S.6. Efficacy predictions using combinations of two 2D pharmacophore parameters with different measures of overlap coefficients. The recalculated OC parameters for **17** with Leu[5] residue (B2) as the hydrophobic B group were used for this analysis.

2D Pharmacophoric Parameters	R^2			
	Centroid	**Centroid=**	**MaxD**	**MaxD=**
AB-NBA + AB-ANB	0.704	0.539	**0.927**	0.605
AB-NBA + AB-NAB	0.351	0.412	**0.944**	0.534
AB-NBA + BN-ANB	0.646	0.394	**0.932**	0.529
AB-NBA + BN-NAB	0.700	0.614	**0.942**	0.576
AB-NBA + BN-NBA	0.692	0.738	**0.949**	0.590
AB-NBA + NA-ANB	0.480	0.415	0.830	0.582
AB-NBA + NA-NAB	0.564	0.523	0.827	0.557
AB-NBA + NA-NBA	0.741	0.792	**0.978**	0.891

Table S.7. Efficacy predictions using combinations of two 2D pharmacophore parameters with different measures of overlap coefficients. **7** was used as the reference compound in the calculations of OC.

	R^2			
2D Pharmacophoric Parameter	**Centroid**	**Centroid=**	**MaxD**	**MaxD=**
AB-NBA + AB-ANB	0.869	0.410	**0.902**	0.590
AB-NBA + AB-NAB	0.413	0.277	**0.908**	0.504
AB-NBA + BN-ANB	0.743	0.278	**0.910**	0.416
AB-NBA + BN-NAB	0.821	0.593	**0.909**	0.586
AB-NBA + BN-NBA	0.900	0.739	0.859	0.497
AB-NBA + NA-ANB	0.777	0.581	0.738	0.587
AB-NBA + NA-NAB	0.899	0.791	0.762	0.364
AB-NBA + NA-NBA	0.873	0.852	**0.946**	0.750
NA-NBA + AB-ANB	0.875	0.819	**0.958**	0.747
NA-NBA + AB-NAB	0.880	0.820	**0.966**	0.706
NA-NBA + BN-ANB	0.871	0.835	**0.964**	0.713
NA-NBA + BN-NAB	0.872	0.829	**0.965**	0.735
NA-NBA + BN-NBA	0.887	0.840	**0.986**	0.712
NA-NBA + NA-ANB	0.871	0.842	**0.953**	0.735
NA-NBA + NA-NAB	0.887	0.872	**0.968**	0.713

Table S.8. Efficacy predictions using combinations of three 2D pharmacophore parameters with different measures of overlap coefficients. **6** was used as the reference compound in the calculations of OC.

		R^2		
2D Pharmacophoric Parameter	**Centroid**	**Centroid=**	**MaxD**	**MaxD=**
AB-NBA + BN-ANB + NA-NBA	0.343	0.366	0.785	0.856
AB-NBA + BN-NAB + NA-NBA	0.347	0.449	0.763	0.828
AB-NBA + AB-ANB + NA-NBA	0.345	0.428	0.771	0.804
AB-NBA + AB-NAB + NA-NBA	0.675	0.394	0.775	0.867
AB-NBA + NA-ANB + NA-NBA	0.449	0.736	0.773	**0.944**
AB-NBA + NA-NAB + NA-NBA	0.607	0.478	0.720	0.838
NA-NBA + BN-NAB + AB-ANB	0.358	0.472	0.184	0.809
NA-NBA + BN-NAB + AB-NAB	0.427	0.427	0.441	0.891
NA-NBA + BN-NAB + AB-NBA	0.347	0.449	0.763	0.828
NA-NBA + BN-NAB + BN-ANB	0.373	0.482	0.172	0.803
NA-NBA + BN-NAB + BN-NBA	0.170	0.670	0.351	0.882
NA-NBA + BN-NAB + NA-ANB	0.209	0.780	0.344	**0.966**
NA-NBA + BN-NAB + NA-NAB	0.279	0.384	0.144	0.836
NA-NBA + NA-NAB + AB-ANB	0.344	0.436	0.148	0.886
NA-NBA + NA-NAB + AB-NAB	0.453	0.434	0.148	0.821
NA-NBA + NA-NAB + AB-NBA	0.607	0.478	0.720	0.838
NA-NBA + NA-NAB + BN-ANB	0.298	0.480	0.148	0.817
NA-NBA + NA-NAB + BN-NAB	0.279	0.384	0.144	0.836
NA-NBA + NA-NAB + BN-NBA	0.394	0.439	0.455	**0.968**
NA-NBA + NA-NAB + NA-ANB	0.602	0.617	0.849	**0.929**

Table S.9. Overlap coefficients for the pharmacophoric parameters of **18**, using different hydrophobic groups for the pharmacophore group B. The various measurements of overlap coefficients are shown with the values obtained using different B groups labeled as shown below.

$(H_2C{=}CCH_2)_2$-Tyr-Aib-Aib-Phe-Leu
B2 / B3 B1 B4

OC-type	B-type	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
	B1	0.144403	0.261082	0.17106	0.221606	0.103541	0.00876	0.005494	0.006792	0.004183
Centroid	B2	0	0	0.207129	0	0	0	0.000201	0	0.000445
	B3	0	0	0.136602	0	0	0	0	0	0.003076
	B4	0.000011	0.000035	0.000202	0.000018	0.00009	0.00007	0.006047	0.004487	0.00001
	B2-3	0	0	0.06493	0	0	0	0	0	0.00081
	B1	0.178343	0.26133	0.351907	0.21267	0.231234	0.247033	0.209814	0.243117	0.246412
Centroid=	B2	0	0	0.548998	0	0	0	0.108581	0	0.132857
	B3	0	0	0.569817	0	0	0	0	0	0.218977
	B4	0.005464	0.00773	0.078439	0.007453	0.005459	0.063384	0.19727	0.231719	0.09323
	B2-3	0	0	0.29655	0	0	0	0	0	0.16618
	B1	0.055954	0.077196	0.063317	0.072292	0.06584	0.044329	0.060808	0.069865	0.025992
MaxD	B2	0	0	0.002726	0	0	0	0.005106	0	0.025911
	B3	0	0	0.002233	0	0	0	0.000017	0	0.024385
	B4	0.041485	0.021043	0.039248	0.03034	0.039496	0.012082	0.081383	0.075987	0.008317
	B2-3	0	0	0.00226	0	0	0	0.000002	0	0.02489
	B1	0.328594	0.379415	0.385347	0.373331	0.33157	0.341539	0.431171	0.420387	0.292372
MaxD=	B2	0	0	0.138218	0	0	0	0.29951	0	0.219596
	B3	0	0	0.159725	0	0	0	0.049868	0	0.270473
	B4	0.254503	0.23921	0.311222	0.245726	0.257505	0.213277	0.369423	0.415843	0.336027
	B2-3	0	0	0.16384	0	0	0	0.01772	0	0.28692

Table S.10. Efficacy predictions using combinations of two 2D pharmacophore parameters for the MaxD based calculation of OC. Four different groups, Phe[4] (B1), allylic amino groups (B1, B2 & B2-3), Leu[5] (B4) were used for the definition of the pharmacophoric B group in this analysis for **18**.

2D Pharmacophoric Parameter	R^2 B1	B2	B3	B4	B2-3
AB-NBA + AB-ANB	0.688	**0.931**	**0.931**	0.785	**0.931**
AB-NBA + AB-NAB	0.742	**0.947**	**0.947**	**0.879**	**0.947**
AB-NBA + BN-ANB	0.700	**0.937**	**0.937**	0.842	**0.937**
AB-NBA + BN-NAB	0.695	**0.946**	**0.946**	0.822	**0.946**
AB-NBA + BN-NBA	0.782	**0.951**	**0.952**	0.774	**0.952**
AB-NBA + NA-ANB	0.728	0.849	0.850	0.802	0.850
AB-NBA + NA-NAB	0.720	0.844	0.844	0.787	0.844
AB-NBA + NA-NBA	0.727	**0.905**	**0.910**	**0.905**	**0.909**

Table S.11. Overlap Coefficients (OC) of the pharmacophore parameters for the δ opioid ligands with respect to **4** obtained using the centroids of the pharmacophoric groups as pharmacophoric points, i) with sampled probability weighting ii) with equal weighting for all points in conformational space. Different definitions for the hydrophobic B group in **17** and **18** are indicated with the compound number.

i) Centroid

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
1	0	0.079188	0.000068	0.000033	0	0	0.012717	0.003073	0
2	0	0	0	0	0	0	0	0	0.000003
3	0	0	0	0	0	0	0	0	0.074961
4	1	1	1	1	1	1	1	1	1
5	0.9992	0.997443	0.996095	0.999102	0.998348	0.996672	0.9955	0.995601	0.996654
6	0.003193	0.003532	0.005945	0.002898	0.002602	0.010281	0.016834	0.0967	0.011091
7	0	0.048341	0.000005	0.002387	0	0	0.000582	0.000004	0
8	0.000529	0.000371	0.000333	0.000536	0.000449	0.008716	0.000863	0.00105	0.036227
9	0.993379	0.993254	0.994837	0.993125	0.993281	0.998909	0.997245	0.998471	0.998472
14	0.000703	0.000337	0.000066	0.000422	0.000781	0.000001	0.000915	0.002287	0.000002
15	0.265787	0.310746	0.146626	0.263123	0.192035	0.048982	0.018665	0.017821	0.010481
16	0.231582	0.201463	0.147881	0.21944	0.162016	0.05419	0.027665	0.028043	0.016655
17	0.000147	0.000287	0.048409	0.000184	0.000411	0.000021	0.000004	0.000005	0.001479
17-B2	0.020821	0.014038	0.110769	0.012807	0.010746	0.040935	0.041905	0.01251	0.028142
18	0.305473	0.213941	0.136432	0.240415	0.229692	0.04024	0.020115	0.034518	0.017242
18-B2	0	0	0.000639	0	0	0	0.00451	0	0.000139
18-B3	0	0	0.055214	0	0	0	0	0	0.012634
18-B4	0	0	0	0	0	0	0.028041	0.013656	0
18-B2-3	0	0	0.140637	0	0	0	0	0	0.022958

ii) Centroid=

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
1	0	0.416378	0.143666	0.091504	0	0	0.285345	0.219663	0
2	0	0	0.01715	0	0	0	0	0	0.135613
3	0	0	0	0	0	0	0	0	0.732675
4	1	1	1	1	1	1	1	1	1
5	0.929412	0.897083	0.866044	0.933081	0.91291	0.905313	0.915161	0.8965	0.964901
6	0.36802	0.386941	0.477868	0.334318	0.395413	0.474424	0.547473	0.630667	0.573068
7	0	0.395273	0.030376	0.23843	0	0.012671	0.206232	0.057596	0
8	0.176949	0.187321	0.294602	0.156237	0.201057	0.394611	0.248003	0.326207	0.544415
9	0.915929	0.915806	0.898249	0.902004	0.913043	0.88426	0.894475	0.902973	0.931034
14	0.045645	0.024967	0.0291	0.037132	0.060068	0.010238	0.143402	0.211652	0.021041
15	0.115172	0.153013	0.189341	0.121944	0.130708	0.142615	0.183716	0.218475	0.171065
16	0.104071	0.134218	0.179708	0.107254	0.114889	0.124114	0.192079	0.217982	0.159007
17	0.025687	0.028096	0.167334	0.020594	0.033807	0.027778	0.022697	0.032057	0.164861
17-B2	0.103952	0.132784	0.171291	0.106784	0.115942	0.121082	0.202326	0.237051	0.161709
18	0.096058	0.113873	0.168157	0.098273	0.097828	0.142344	0.216748	0.230022	0.189567
18-B2	0	0	0.157464	0	0	0	0.190867	0	0.087637
18-B3	0	0	0.263935	0	0	0	0	0	0.172818
18-B4	0	0	0.001987	0	0	0.00261	0.206096	0.215985	0
18-B2-3	0	0	0.226832	0	0	0	0	0	0.153674

Table S.12. Overlap Coefficients (OC) of the pharmacophore parameters for the δ opioid ligands with respect to **4** obtained using the most distant atoms between the pharmacophoric groups, A and B as pharmacophore points, i) with sampled probability weighting ii) with equal weighting for all points in conformational space. Different definitions for the hydrophobic B group in **17** and **18** are indicated with the compound number.

i) MaxD

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
1	0	0.000297	0.000996	0.001162	0.000008	0.000069	0.050368	0.092267	0
2	0	0	0.0492	0	0	0	0	0	0.092871
3	0	0	0.000001	0	0	0.000099	0	0	0
4	1	1	1	1	1	1	1	1	1
5	0.998144	0.997447	0.996182	0.998497	0.998336	0.998289	0.994872	0.99484	0.99719
6	0.009136	0.002382	0.001976	0.00744	0.005214	0.05046	0.008297	0.020199	0.002768
7	0	0.000023	0.000165	0.001761	0	0.00061	0.002708	0.000632	0
8	0.000651	0.000026	0.000341	0.000198	0.00015	0.000527	0.000143	0.00011	0.008698
9	0.990065	0.994663	0.997533	0.995303	0.990823	0.995592	0.996676	0.996817	0.996455
14	0.093061	0.04515	0.032653	0.07044	0.062849	0.052161	0.057448	0.056057	0.0304
15	0.080481	0.129881	0.092059	0.084626	0.068954	0.090706	0.032777	0.02786	0.064724
16	0.170757	0.070597	0.081941	0.148518	0.074903	0.085747	0.094005	0.087233	0.035226
17	0.000203	0.000119	0	0.000131	0.000084	0	0.000037	0.000043	0
17-B2	0.003827	0.002473	0.068911	0.001865	0.001653	0.002716	0.066881	0.019242	0.072754
18	0.11398	0.094003	0.130703	0.096499	0.091896	0.123961	0.277686	0.240881	0.11175
18-B2	0	0	0.12348	0	0	0	0.003521	0	0.002206
18-B3	0	0	0.060117	0	0	0	0	0	0.004001
18-B4	0.00018	0.00017	0.001327	0.000076	0.000118	0.001404	0.226103	0.242291	0.000253
18-B2-3	0	0	0.063508	0	0	0	0	0	0.004312

ii) MaxD=

Compound	AB-ANB	AB-NAB	AB-NBA	BN-ANB	BN-NAB	BN-NBA	NA-ANB	NA-NAB	NA-NBA
1	0.006042	0.121844	0.212793	0.203099	0.022993	0.112956	0.401597	0.387985	0
2	0	0	0.343025	0	0	0	0	0	0.58191
3	0	0	0.015293	0	0	0.095507	0	0	0.028028
4	1	1	1	1	1	1	1	1	1
5	0.910909	0.901773	0.910539	0.88983	0.912037	0.887037	0.909768	0.8989	0.880597
6	0.480128	0.46239	0.500997	0.530093	0.486971	0.621849	0.50942	0.554314	0.572281
7	0	0.037809	0.122084	0.177891	0.002017	0.210733	0.366864	0.2346	0
8	0.20884	0.091803	0.188357	0.146619	0.11738	0.281838	0.14694	0.136077	0.401098
9	0.906943	0.894354	0.908654	0.876874	0.897235	0.901695	0.902181	0.89748	0.931542
14	0.181453	0.235853	0.258008	0.186091	0.209678	0.225637	0.254003	0.298019	0.229333
15	0.171824	0.223751	0.265534	0.184907	0.191614	0.213687	0.267372	0.296925	0.209331
16	0.145416	0.177883	0.243675	0.148284	0.151499	0.175863	0.264145	0.282767	0.190822
17	0.020584	0.031145	0	0.015931	0.035608	0	0.035413	0.035301	0
17-B2	0.1144	0.153207	0.236652	0.115512	0.12337	0.152402	0.27726	0.235328	0.189235
18	0.138974	0.159235	0.227241	0.141147	0.137229	0.191977	0.300047	0.314962	0.206909
18-B2	0	0	0.316965	0	0	0	0.234035	0	0.174104
18-B3	0	0	0.35871	0	0	0	0.002458	0	0.199814
18-B4	0.013952	0.012042	0.10219	0.009906	0.01226	0.079436	0.294924	0.299598	0.080135
18-B2-3	0	0	0.375375	0	0	0	0	0	0.211962